

(1,3-¹³C₂)Propan-2-ol
117072-72-7 | DTXSID90745872

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.07

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 8.46e-01

Nearest Neighbors from the Training Set

Image not found

tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

Image not found

Dimethyl sulfoxide

Measured: 3.98

Predicted: 4.07

Image not found

Diethyl ether

Measured: 5.37

Predicted: 4.72

Image not found

3-Pyridinamine

Measured: 2.09

Predicted: 3.04

Image not found

4-Aminopyridine

Measured: 4.57

Predicted: 3.04